AD-A142 555 RARE-EARTH ION-HOST LATTICE INTERACTIONS: 15 ANALYSIS OF THE SPECTRA OF ND3+ IN GD3SC2GA3O12(U) HARRY DIAMOND LABS ADELPHI MD C A MORRISON ET AL. MAY 84 HDL-TR-2035 1/1

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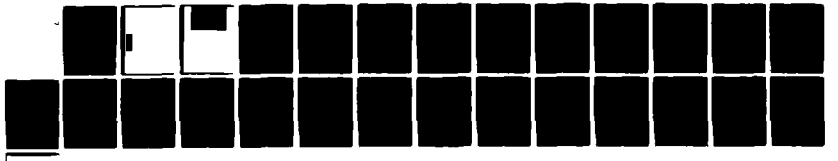

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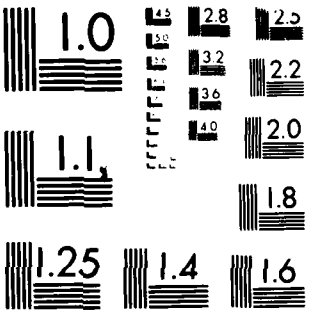

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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

The Judd-Ofelt theory of induced electric-dipole transitions is used to calculate multiplet-to-multiplet line strengths, lifetimes, and branching ratios, and line-to-line squared matrix elements between all the energy levels considered for the triply ionized lanthanides Ce^{3+} through Yb^{3+} in $Gd_3Sc_2Ga_3O_{12}$. Magnetic-dipole transitions are also calculated. The even-n B_{nm} used in the calculations are obtained by smoothing the phenomenological B_{nm} obtained by fitting experimental data on neodymium. The odd-n A_{nm} are obtained from appropriate lattice sums. These results are compared with neodymium in several popular host materials. Detailed intensity

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20. ABSTRACT (Cont'd)

calculations (line to line) and g-factor calculations have been performed and the results are attached in microfiche form.

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1. INTRODUCTION

The material $Gd_3Sc_2Ga_3O_{12}$ is a mixed garnet with the same crystal structure as the popular laser material $Y_3Al_5O_{12}$ (YAG).[1,2] The chemical formula for YAG is sometimes written as $Y_3Al_2Al_3O_{12}$ to illustrate that two types of aluminum sites exist in this material. In the material $Gd_3Sc_2Ga_3O_{12}$ each ion type occupies a single site type. The optical spectra and laser action of Nd^{3+} in $Gd_3Sc_2Ga_3O_{12}$ have been reported by Kaminskii.[3,4] An interesting feature of this material is that if it is doped with both Nd^{3+} and Cr^{3+}, energy is transferred efficiently from the Cr^{3+} to the Nd^{3+} impurities.[5] The microwave phonon attenuation of this and related garnets has been measured at a number of different temperatures.[6] The indices of refraction of a number of related mixed rare-earth garnets[7] have been measured in the wavelength region from 5200 to 6200 Å. Although the optical spectra of only one rare-earth ion in this host, Nd^{3+}, have been reported, we considered the host important enough to do a preliminary crystal-field analysis of rare-earth ions.

In this report we use techniques reported previously[8,9] to obtain first estimates of the crystal-field parameters for $Nd:Gd_3Sc_2Ga_3O_{12}$. These parameters are used as starting values in a program that varies the crystal-field parameters to obtain a best least-squares fit to the experimental data. The resulting crystal-field parameters are used in conjunction with odd-fold lattice sums to obtain the Judd-Ofelt intensity parameters, the level-to-level line strengths for electric- and magnetic-dipole transitions, and the branching ratios for the entire rare-earth series. Comparisons to corresponding calculations on other host materials are made throughout.

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[1] *M. J. Weber, Handbook of Lasers, Chemical Rubber Company, Cleveland, Ohio (1971), chapter 13, p 371.*

[2] *C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials, in Handbook on the Physics and Chemistry of Rare Earths, Vol 5, K. A. Gschneidner and L. Eyring, Jr., eds., North Holland, New York (1982), p 632.*

[3] *A. A. Kaminskii, Kh. S. Bagdasarov, G. A. Bogomolova, M. M. Gritsenko, A. M. Kevorkov, and S. E. Sarkisov, Luminescence and Stimulated Emission of Nd^{3+} Ions in $Gd_3Sc_2Ga_3O_{12}$ Crystals, Phys. Stat. Sol. (a) 34 (1976), K109.*

[4] *A. A. Kaminskii, Laser Crystals, Springer-Verlag, New York (1981), p 133.*

[5] *D. Pruss, G. Huber, A. Biemowski, V. V. Laptev, I. A. Shcherbakov, and Y. V. Zharikov, Efficient Cr^{3+} Sensitized Nd^{3+}:GdScGa--Garnet Laser at 1.06 μm, Appl. Phys. B28 (1982), 358. See also E. V. Zharikov, V. V. Laptev, E. I. Sidorova, Yu. P. Timefeev, and I. A. Shcherbakov, Absolute Quantum Efficiency of the Luminescence of Cr^{3+} Ions in Gadolinium Gallium and Gadolinium Scandium Gallium Garnet Crystals, Sov. J. Quant. Electron. 12 (1982), 1124.*

[6] *M. Dutoit, J. C. Walling, and D. S. Boudreaux, Microwave Phonon Attenuation in Rare-Earth Garnets: Ion-Phonon Interactions, Phys. Rev. B11 (1975), 349.*

[7] *S. H. Wemple and W. J. Tabor, Refractive Index Behavior of Garnets, J. Appl. Phys. 44 (1973), 1395.*

[8] *C. A. Morrison and R. P. Leavitt, Crystal Field Analysis of Triply Ionized Rare Earth Ions in Lanthanum Trifluoride, J. Chem. Phys. 71 (1979), 2366.*

[9] *R. P. Leavitt and C. A. Morrison, Crystal Field Analysis of Triply Ionized Rare Earth Ions in Lanthanum Trifluoride. II. Intensity Calculations, J. Chem. Phys. 73 (1980), 749.*

2. CRYSTAL FIELD

The crystallographic data[10] on $Gd_3Sc_2Ga_3O_{12}$ are given in table 1. We were unable to find a refined x-ray study of this material and have taken the oxygen positions to be the same as reported for $Y_3Ga_5O_{12}$. The lattice sums, A_{nm}, were evaluated using these x-ray data. Effective charges, Z_i ($q_i = eZ_i$), in units of the magnitude of the electron charge, were taken as $Z_{Gd} = Z_{Sc} = 3$, $Z_{Ga} = 1$, and $Z_O = -1.5$. The resulting point-charge contributions to the A_{nm} are shown in column 2 of table 2. The point-dipole[11] and self-induced[12] contributions to the A_{nm} were also evaluated and are shown in columns 3 and 4. In the evaluation of these latter contributions, the polarizability of oxygen was taken to be one-tenth of the handbook value (based on previous experience). The point-charge contributions to the A_{nm} for the isostructural materials $Y_3Al_5O_{12}$[13] and $Y_3Ga_5O_{12}$[14] are included in table 3 for comparison.

TABLE 1. CRYSTALLOGRAPHIC DATA FOR $Gd_3Sc_2Ga_3O_{12}$
(CUBIC SPACE GROUP Ia3d, No. 230, Z = 8)[a]

Ion	Position	Symmetry	x	y	z
Gd	24(c)	D_2	0	1/4	1/8
Sc	16(a)	C_{3i}	0	0	0
Ga	24(d)	S_4	3/8	0	1/4
O	96(h)	C_1	-0.0272	0.0558	0.1501

[a] *Fractional oxygen positions are from isostructural material $Y_3Ga_5O_{12}$ (Morrison and Leavitt, ref 2, p 643). Lattice constant is a = 12.5668 Å (Brandle and Barns, ref 10).*

[10] *C. D. Brandle and R. L. Barns, Crystal Stoichiometry and Growth of Rare-Earth Garnets Containing Scandium, J. Cryst. Growth 20 (1979), 1.*

[11] *C. A. Morrison, Dipolar Contributions to the Crystal Field in Ionic Solids, Solid State Commun. 18 (1976), 153.*

[12] *C. A. Morrison, G. F. de Sá, and R. P. Leavitt, Self-Induced Multipole Contribution to the Single-Electron Crystal Field, J. Chem. Phys. 76 (1982), 3899.*

[13] *D. E. Wortman, C. A. Morrison, and N. Karayianis, Rare Earth Ion-Host Lattice Interactions: 11. Lanthanides in $Y_3Al_5O_{12}$, Harry Diamond Laboratories, HDL-TR-1773 (August 1976).*

[14] *N. Karayianis, D. E. Wortman, and C. A. Morrison, Rare Earth Ion-Host Lattice Interactions: 12. Lanthanides in $Y_3Ga_5O_{12}$, Harry Diamond Laboratories, HDL-TR-1793 (July 1977).*

TABLE 2. POINT-CHARGE, POINT-DIPOLE, AND SELF-INDUCED LATTICE SUMS A_{nm} ($cm^{-1}/Å^n$), FOR $Gd_3Sc_2Ga_3O_{12}$

A_{nm}	Point-charge[a]	Point-dipole[b]	Self-induced[b]	Total
A_{20}	4616.	-1006.	-38.42	3572.
A_{22}	2294.	-1324.	39.44	1010.
A_{32}	i224.5	-i679.5	i51.47	-i403.6
A_{40}	224.1	-234.4	2.043	-8.190
A_{42}	-4142.	-56.08	208.6	-3990.
A_{44}	-2130.	-133.7	122.2	-2141.
A_{52}	-i1602.	-i19.33	i106.5	-i1515.
A_{54}	i979.0	i22.26	-i58.05	i943.2
A_{60}	-1036.	-26.88	82.22	-981.1
A_{62}	-406.6	17.89	38.58	-350.1
A_{64}	528.4	20.26	-44.30	504.4
A_{66}	-401.0	29.17	35.10	-336.8
A_{72}	i61.01	i4.051	-i7.057	i58.01
A_{74}	i150.1	i32.29	-i21.02	i161.4
A_{76}	-i151.5	-i8.299	i13.14	-i146.6

[a] *X-ray data are given in table 1. Effective charges are* $Z_{Gd} = +3$, $Z_{Sc} = +3$, $Z_{Ga} = +1$, *and* $Z_O = -1.5$.

[b] *Polarizability of oxygen,* α_O, *is taken to be 0.244* $Å^3$.

TABLE 3. POINT-CHARGE LATTICE SUMS A_{nm} ($cm^{-1}/Å^n$) FOR $Y_3Al_5O_{12}$ AND $Y_3Ga_5O_{12}$

A_{nm}	$Y_3Al_5O_{12}$[a]	$Y_3Ga_5O_{12}$[b]
A_{20}	1453	4948.
A_{22}	2292	2459.
A_{32}	-i2758	i246.2
A_{40}	-614.6	?51.6
A_{42}	-4916	-4649.
A_{44}	-2799	-2390.
A_{52}	-i2015	-i1840.
A_{54}	i1159	i1125.
A_{60}	-1481	-1218.
A_{62}	-568.2	-477.9
A_{64}	546.2	621.1
A_{66}	-503.1	-471.4
A_{72}	i30.62	i73.38
A_{74}	i84.41	i180.6
A_{76}	-i176.2	-i182.2

[a] *X-ray data were taken from Morrison and Leavitt (ref 2, p 634). Effective charges are* $Z_Y = +3$, $Z_{Al} = +1.92$, *and* $Z_O = -1.55$.

[b] *X-ray data were taken from Morrison and Leavitt (ref 2, p 643). Effective charges are* $Z_Y = +3$, $Z_{Ga_1} = +3$, $Z_{Ga_2} = +1$, *and* $Z_O = -1.5$.

The A_{nm} of column 2 of table 2 were used to calculate crystal-field parameters B_{nm} for neodymium using

$$B_{nm} = \rho_n(Nd)A_{nm} \quad , \qquad (1)$$

where the ρ_n(Nd) are radial factors given in an earlier work.[15] These B_{nm} were then used as initial values in a least-squares fit to the experimental data on ND:$Gd_3Sc_2Ga_3O_{12}$. The best fit for all the reported data was extremely poor, and the resultant B_{nm} were far from those obtained for Nd^{3+} in the isostructural compounds $Y_3Al_5O_{12}$ and $Y_3Ga_5O_{12}$. These results are shown in table 4.

TABLE 4. BEST FIT OF CALCULATED ENERGY LEVELS TO EXPERIMENTAL ENERGY LEVELS OF Nd:$Gd_3Sc_2Ga_3O_{12}$ USING ALL EXPERIMENTAL DATA OF KAMINSKII ET AL (ref 3, 4) (E = experimental, T = theoretical)[a]

Term		Prefix[b]	Energy (cm^{-1})						
$^4I_{9/2}$	E	-	0	107	168	263	763		
	T	-	-84	136	201	304	746		
$^4I_{11/2}$	E	1	978	010*	069	109	393	431	
	T	2	000	023	067	112	339	443	
$^4I_{13/2}$	E	3	907	920	000*	010	025	380	421
	T	3	890	900	933	013*	192	337	406
$^4I_{15/2}$	E	5	777	812	914	959	494*	510	557
	T	5	772	812	915	009*	431	474	591
	E	6	647						
	T	6	664						
$^4F_{3/2}$	E	11	434	499					
	T	11	434	494					

[a] *Rms deviation is 45.95 cm^{-1}. Resulting B_{nm} (cm^{-1}) are B_{20} = 187, B_{22} = -273, B_{40} = -390, B_{42} = -475, B_{44} = -2157, B_{60} = -2081, B_{62} = -307, B_{64} = 706, and B_{66} = -211.*

[b] *Prefix for entries to right. Asterisk indicates that, for that entry and succeeding entries in that row, prefix is increased by one. Thus for experimental data in $^4I_{11/2}$ we have*

1 978 010 069 ... = 1978 2010 2069 ...*

[15] *C. A. Morrison, N. Karayianis, and D. E. Wortman, Rare Earth Ion-Host Lattice Interactions: 4. Predicting Spectra and Intensities of Lanthanides in Crystals, Harry Diamond Laboratories, HDL-TR-1816 (June 1977).*

For several reasons, we then chose to remove the level at 4000 cm^{-1} in an attempt to remedy the poor fit. First, our lattice-sum calculation predicts no line in the vicinity of the 4000-cm^{-1} line. Second, examination of the data on Nd^{3+} in other garnets[2] reveals at most four lines below 4200 cm^{-1} within the $^4I_{13/2}$ manifold. Third, Kaminskii et al[3] mention extra lines in their data. Finally, and most importantly, rejection of the 4000-cm^{-1} line leads to a vastly improved fit of the data. The best fit to the experimental data (minus the 4000-cm^{-1} line) was obtained again; results of this fit are shown in table 5. The rms deviation between the calculated and experimental energy levels was very small (~2 cm^{-1}) and represents one of the best fits that we have ever obtained to experimental energy-level data in crystals. Shown in table 6 are the best-fit B_{nm} and the phenomenological A_{nm} (for *even* n) obtained from the best fit B_{nm} by

$$A_{nm} = B_{nm}/\rho_n(Nd) \quad , \tag{2}$$

where $\rho_n(Nd)$ is the same as in equation (1).

TABLE 5. BEST FIT OF CALCULATED ENERGY LEVELS TO EXPERIMENTAL ENERGY LEVELS OF Nd:$Gd_3Sc_2Ga_3O_{12}$ WITH LEVEL AT 4000 cm^{-1} REMOVED FROM EXPERIMENTAL DATA GIVEN IN TABLE 4[a]

Term		Prefix[b]	Energy (cm^{-1})						
$^4I_{9/2}$	E	-	0	107	168	263	763		
	T	-	-1	105	168	267	762		
$^4I_{11/2}$	E	1	978	010*	069	109	393	431	
	T	1	979	006*	070	107	394	435	
$^4I_{13/2}$	E	3	907	920	010*	025	-	380	421
	T	3	911	923	009*	020	367	381	419
$^4I_{15/2}$	E	5	777	812	914	959	494*	510	557
	T		777	809	916	962	495*	512	557
	E	6	647						
	T	6	643						
$^4F_{3/2}$	E	11	434	499					
	T	11	435	498					

[a] *Rms is 2.37 cm^{-1}. Resulting best-fit B_{nm} are given in table 6.*
[b] *For explanation of notation, see footnotes of table 4.*

[2] *C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials, in Handbook on the Physics and Chemistry of Rare Earths, Vol 5, K. A. Gschneidner and L. Eyring, Jr., eds., North Holland, New York (1982), p 632.*

[3] *A. A. Kaminskii, Kh. S. Bagdasarov, G. A. Bogomolova, M. M. Gritsenko, A. M. Kevorkov, and S. E. Sarkisov, Luminescence and Stimulated Emission of Nd^{3+} Ions in $Gd_3Sc_2Ga_3O_{12}$ Crystals, Phys. Stat. Sol. (a) 34 (1976), K109.*

TABLE 6. BEST FIT B_{nm} FOR Nd IN $Gd_3Sc_2Ga_3O_{12}$ AND PHENOMENOLOGICAL A_{nm} ($A_{nm} = B_{nm}/\rho_n(Nd)$)

nm	$B_{nm}(cm^{-1})$	$A_{nm}(cm^{-1}/\text{Å}^n)$
20	434	2544
22	90	529
40	-67	-115
42	-1818	-3148
44	-921	-1595
60	-1485	-934
62	-679	-427
64	771	485
66	-661	-416

The A_{nm} obtained by using equation (2), as given in table 6, were then compared to the various contributions to the A_{nm} given in table 2. It is apparent that if different polarizabilities and effective charges were chosen, the values of A_{nm} of table 2 could be brought into better agreement with those of table 6. However, because of the lack of refined x-ray data for $Gd_3Sc_2Ga_3O_{12}$ (that is, the oxygen positions are unknown), no attempt was made to investigate such changes. The phenomenological A_{nm} of table 6 for even n were used in equation (1) to obtain B_{nm} for the entire rare-earth series. These B_{nm} are given in table 7.

TABLE 7. SMOOTHED CRYSTAL-FIELD PARAMETERS B_{nm} (cm^{-1}) FOR ALL RARE-EARTH IONS R^{3+} FOR R:$Gd_3Sc_2Ga_3O_{12}$

R	B_{20}	B_{22}	B_{40}	B_{42}	B_{44}	B_{60}	B_{62}	B_{64}	B_{66}
Ce	468	97.5	-86.8	-2372	-1202	-2187	-1000	1136	-974
Pr	447	93.0	-74.4	-2035	-1031	-1752	-801	910	-780
Nd	434	90.3	-66.5	-1818	-921	-1485	-679	771	-661
Pm	427	88.9	-61.5	-1680	-851	-1328	-607	690	-591
Sm	424	88.3	-58.1	-1589	-805	-1234	-564	641	-549
Eu	424	88.2	-55.7	-1522	-771	-1168	-534	606	-520
Gd	424	88.3	-53.6	-1465	-742	-1109	-507	576	-494
Tb	426	88.6	-51.7	-1413	-716	-1049	-480	545	-467
Dy	428	89.0	-50.0	-1366	-692	-991	-453	515	-441
Ho	430	89.6	-48.6	-1327	-672	-945	-432	491	-421
Er	434	90.3	-47.5	-1299	-658	-918	-420	477	-409
Tm	438	91.2	-46.7	-1276	-646	-901	-412	468	-401
Yb	442	91.9	-45.3	-1239	-628	-852	-390	442	-379

The *odd*-n A_{nm} given in column 2 of table 2 were used to calculate the Judd-Ofelt intensity parameters, Ω_k, for all the rare-earth ions in $Gd_3Sc_2Ga_3O_{12}$. The Ω_k are given in table 8. In table 9 the corresponding Ω_k are calculated for R:$Y_3Al_5O_{12}$ and in table 10 the Ω_k are given for R:$LiYF_4$. The results in tables 9 and 10 are included here for comparison.

TABLE 8. CALCULATED JUDD-OFELT INTENSITY PARAMETERS FOR R:$Gd_3Sc_2Ga_3O_{12}$[a]

R	Ω_2 (10^{-20} cm^2)	Ω_4 (10^{-20} cm^2)	Ω_6 (10^{-20} cm^2)
Ce	12.75	2.817	26.21
Pr	7.136	1.423	11.19
Nd	6.880	0.8867	6.139
Pm	3.982	0.6923	4.717
Sm	3.472	0.5808	3.903
Eu	2.747	0.4554	2.764
Gd	2.150	0.3540	1.909
Tb	3.754	0.5356	4.615
Dy	2.761	0.3963	2.866
Ho	2.255	0.3210	2.093
Er	2.162	0.2998	1.974
Tm	2.103	0.2846	1.906
Yb	1.774	0.2360	1.452

[a]*Odd-n A_{nm} used in calculation of Ω_k are from column 2 of table 2.*

TABLE 9. CALCULATED JUDD-OFELT INTENSITY PARAMETERS FOR R:$Y_3Al_5O_{12}$[a]

R	Ω_2 (10^{-20} cm^2)	Ω_4 (10^{-20} cm^2)	Ω_6 (10^{-20} cm^2)
Ce	1.933	8.751	39.78
Pr	1.082	4.413	16.96
Nd	1.043	2.855	9.293
Pm	0.6036	2.197	7.147
Sm	0.5264	1.871	5.864
Eu	0.4165	1.422	4.186
Gd	0.3259	1.065	2.887
Tb	0.5692	2.066	7.029
Dy	0.4186	1.422	4.360
Ho	0.3418	1.112	3.181
Er	0.3278	1.057	3.001
Tm	0.3188	1.023	2.899
Yb	0.2690	0.8288	2.208

[a]*Odd-fold A_{nm} used in calculation of Ω_k are from column 2 of table 3.*

The odd A_{nm} of column 2 of table 2 were also used to calculate the line-to-line transition probabilities for electric-dipole and magnetic-dipole transitions for all the rare-earth ions, R^{3+}, in R:$Gd_3Sc_2Ga_3O_{12}$. Also, the branching ratios and g-factors were calculated. These results are included in the form of microfiche copies of computer outputs, at the end of the report; these computer outputs are explained in appendix A. The branching ratios for $^4F_{3/2}$ to ^4I_J for J = 15/2, 13/2, 11/2, and 9/2 are shown in figure 1 for Nd^{3+} in $Y_3Al_5O_{12}$ (YAG), $LiYF_4$(YLF), and $Gd_3Sc_2Ga_3O_{12}$. Results for Nd^{3+} in YAG and YLF are included because experimental data are available for these host materials. It is apparent that the calculated results agree well with the experimental results; this gives further confidence in the accuracy of the calculations on $Gd_3Sc_2Ga_3O_{12}$. Thus, if the x-ray positions assumed for $Gd_3Sc_2Ga_3O_{12}$ are a good approximation, we should expect the results shown in figure 1 for Nd^{3+} in this host to be quite accurate.

TABLE 10. CALCULATED JUDD-OFELT INTENSITY PARAMETERS FOR R:$LiYF_4$[a]

R	$\Omega_2(10^{-20}cm^2)$	$\Omega_4(10^{-20}cm^2)$	$\Omega_6(10^{-20}cm^2)$
Ce	22.28	6.161	52.72
Pr	12.47	3.111	22.48
Nd	12.02	1.949	12.33
Pm	6.956	1.519	9.476
Sm	6.066	1.277	7.845
Eu	4.799	0.9967	5.551
Gd	3.755	0.7706	3.830
Tb	6.559	1.213	9.304
Dy	4.824	0.8864	5.773
Ho	3.939	0.7139	4.213
Er	3.777	0.6686	3.975
Tm	3.673	0.6367	3.839
Yb	3.100	0.5260	2.924

[a] *Even-n B_{nm} are from D. E. Wortman, N. Karayianis, and C. A. Morrison, Rare Earth Ion-Host Lattice Interactons: 6. Lanthanides in $LiYF_4$, Harry Diamond Laboratories, HDL-TR-1770 (August 1976). Odd-n A_{nm} are from L. Esterowitz, F. J. Bartoli, R. E. Allen, D. E. Wortman, C. A. Morrison, and R. P. Leavitt, Energy Levels and Line Intensities of Pr^{3+} in $LiYF_4$, Phys. Rev. B19 (1979), 6442.*

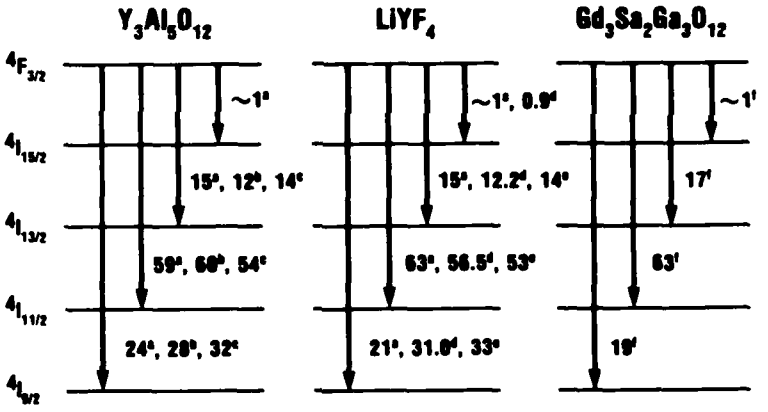

Figure 1. Multiplet-to-multiplet fluorescence branching ratios (in percent) for transitions originating at the $^4F_{3/2}$ level for Nd^{3+} in various hosts:

a, calculated, K. K. Deb, R. G. Buser, C. A. Morrison, and R. P. Leavitt, Crystal Fields and Intensities of Triply Ionized Rare-Earth Ions in Cubic Lanthanum Oxyfluoride: An Efficient $^4F_{3/2} \rightarrow {}^4I_{9/2}$ LaOF:Nd Laser, J. Opt. Soc. Am. 71 (1981), 1463;

b, experimental, R. K. Watts, Jr., Branching Ratios for YAlG:Nd^{3+}, J. Opt Soc. Am. 61 (1971), 123;

c, experimental, S. Singh, R. G. Smith, and L. G. Van Uitert, Stimulated Emission Cross Section and Fluorescent Quantum Efficiency of Nd^{3+} in Yttrium Garnet at Room Temperature, Phys. Rev. B10 (1974), 2566;

d, experimental, H. P. Jenssen, Center for Materials Science and Engineering and Department of Electrical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139 (personal communication);

e, experimental, T. L. Lomheim and L. G. DeShazer, New Procedure of Determining Neodymium Fluorescence Branching Ratios as Applied to 25 Crystals and Glass Hosts, Opt. Commun. 24 (1978), 89;

f, calculated, this work.

3. SCANDIUM AND GALLIUM SITES

To investigate the possibility of other site occupancy by Nd^{3+} or other ions in $Gd_3Sc_2Ga_3O_{12}$, the distances between ions and the number of ion pairs at a given distance were calculated for all the sites in this compound. The results are given in table 11. The ionic radii of several ions in different coordination are given in table 12. The coordination number (CN), the number of nearest ions, for the Gd site is assumed to be 8, since the two groups of oxygen are nearly the same (see table 11) and the next set of ions is much further away (~3.14 Å). The ionic radii of Nd^{3+} and Gd^{3+} for CN = 8 are nearly the same, so we should expect the Nd^{3+} to predominantly enter the Gd^{3+} site in $Gd_3Sc_2Ga_3O_{12}$. However, it is possible that some of the Nd^{3+} may enter the Sc^{3+} site in this compound. For this reason, the point-charge lattice sums A_{nm} were calculated for the Sc^{3+} site in $Gd_3Sc_2Ga_3O_{12}$; the results are given in table 13. Also included in table 13 are the B_{nm} for Nd^{3+} calculated using equation (1). In these calculations, the effective charges on the ions are the same as used in the calculation of table 2. The crystal-field parameters, B_{nm}, for Nd^{3+} in the scandium site as given in table 13 are unrealistically large. This possibly is due to the inaccuracies in the x-ray data. No further calculation was done using the B_{nm} for the scandium site.

TABLE 11. DISTANCE TO NEAREST OXYGEN IONS, R (Å), AND NUMBER OF OXYGEN IONS AT THAT DISTANCE FOR METAL SITES IN $Gd_3Sc_2Ga_3O_{12}$[a]

Site	R	Number	R	Number
Gd	2.39	4	2.48	4
Sc	2.04	6	-	-
Ga	1.89	4	-	-

[a] *X-ray data used are given in table 1.*

TABLE 12. IONIC RADII (Å) AND COORDINATION NUMBERS (CN) OF SEVERAL IONS[a]

Ion	Ionic radius	CN
Gd^{3+}	1.06	8
Nd^{3+}	1.12	8
Sc^{3+}	.87	6
Ga^{3+}	.47	4
Cr^{3+}	.615	6[b]

[a] *R. D. Shannon and C. T. Prewitt, Effective Ionic Radii in Oxides and Fluorides, Acta. Cryst. B25 (1969), 925. Ionic radius is based on oxygen ion in 6 coordination having value 1.40 Å.*

[b] *Ionic radius of Cr^{3+} in 4 coordination is not given in above reference.*

TABLE 13. POINT-CHARGE LATTICE SUMS A_{nm} (cm^{-1}/A^n) FOR Sc^{3+} SITE IN $Gd_3Sc_2Ga_3O_{12}$

nm	A_{nm} [a]	$B_{nm}(Nd)$ [b]
20	812	139
40	-11413	-6592
43	13327	7698
60	666	1058
R 63	2099	3336
I 63	52	83
R 66	687	1092
I 66	25	39

[a] *X-ray data used are given in table 1. Effective charges on ions are as in table 2. Lattice sum was performed for Sc^{3+} site at (0,0,0), and a rotation was performed so that C_{3i} axis is along a body diagonal. Euler angles used are $\alpha = -45°$, $\beta = -54.736°$, and $\gamma = 28.319°$.*
[b] *$B_{nm}(Nd)$ are calculated using equation (1).*

The point-charge lattice sums were calculated for the Ga site (S_4 symmetry) in $Gd_3Sc_2Ga_3O_{12}$; the results are given in table 14. It is highly unlikely that the Nd^{3+} enters this site, because of the large mismatch in ionic radii as given in table 12. However it is quite possible that Cr^{3+} doped in this crystal, as reported elsewhere,[5] may enter this site or perhaps the Sc^{3+} site (see table 12). If the Cr^{3+} were to enter the Ga site substitutionally, the absorption should be quite intense because of the odd-n A_{nm} present in S_4 symmetry. Thus it would be possible to easily pump the Cr^{3+} ion and observe the transfer from Cr^{3+} to a substitutional rare-earth impurity in $Gd_3Sc_2Ga_3O_{12}$. In future work, we expect to use the results in table 14 to estimate the splittings of levels of Cr^{3+} in this host.

TABLE 14. POINT-CHARGE LATTICE SUMS A_{nm} (cm^{-1}/A^n) FOR Ga^{3+} SITE IN $Gd_3Sc_2Ga_3O_{12}$

nm	A_{nm} [a]
20	739
R 32	24281
I 32	-608
40	-13749
44	5515
R 5	2882
I 52	-67
60	-88
R 64	3459
I 64	-285
R 72	-1364
I 72	48
R 76	956
I 76	-121

[a] *X-ray data used are given in table 1. Effective charges on ions are as in table 2. Lattice sum was performed for Ga^{3+} site at (0,0,0), and a rotation was performed so that S_4 axis is along z axis. Euler angles used are $\alpha = 0°$, $\beta = 90°$, and $\gamma = 59.5628°$.*

[5] *D. Pruss, G. Huber, A. Biemowski, V. V. Laptev, I. A. Shcherbakov, and Y. V. Zharikov, Efficient Cr^{3+} Sensitized Nd^{3+}:GdScGa--Garnet Laser at 1.06 μm, Appl. Phys. B28 (1982), 358. See also E. V. Zharikov, V. V. Laptev, E. I. Sidorova, Yu. P. Timefeev, and I. A. Shcherbakov, Absolute Quantum Efficiency of the Luminescence of Cr^{3+} Ions in Gadolinium Gallium and Gadolinium Scandium Gallium Garnet Crystals, Sov. J. Quant. Electron. 12 (1982), 1124.*

4. CONCLUSION

We have analyzed the experimental spectra of Nd^{3+} in the host $Gd_3Sc_2Ga_3O_{12}$. By omitting one of the reported energy levels we were able to obtain an excellent fit (rms $\approx$ 2 cm^{-1}) to the experimental data. The resulting phenomenological crystal-field parameters, B_{nm}, were used to obtain B_{nm} for the entire rare-earth series.[8] Point-charge lattice sums A_{nm} were calculated for effective charges of Z_O = -1.5, Z_{Ga} = +1, Z_{Sc} = +3, and Z_{Gd} = +3. The even-n B_{nm} calculated as in earlier work[2] agreed quite reasonably with the phenomenological B_{nm} obtained by fitting the experimental data. The odd-n A_{nm} from the point-charge lattice sums were used along with the phenomenological B_{nm} to calculate the crystal-field-split energy levels, transition intensities, branching ratios, g values, and lifetimes for the low-lying energy levels of all the rare-earth ions in the Gd^{3+} sites in $Gd_3Sc_2Ga_3O_{12}$. The resulting branching ratios for Nd^{3+} and several other computed quantities were compared with standard laser-host materials (YAG, YLF) with few striking differences. The laser advantages of the garnet $Gd_3Sc_2Ga_3O_{12}$ appear to lie in the fact that the material can be easily doped with transition elements such as Cr^{3+} and still produce high-optical-quality crystals.

Acknowledgement

We wish to thank Jeffrey Paul of NVEOL for suggesting an analysis of the spectra of rare-earth ions in this material and for providing financial support.

[2] *C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials, in Handbook on the Physics and Chemistry of Rare Earths, Vol 5, K. A. Gschneidner and L. Eyring, Jr., eds., North Holland, New York (1982), p 632.*

[8] *C. A. Morrison and R. P. Leavitt, Crystal Field Analysis of Triply Ionized Rare Earth Ions in Lanthanum Trifluoride, J. Chem. Phys. 71 (1979), 2366.*

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(2) C. A. Morrison and R. P. Leavitt, Spectroscopic Properties of Triply Ionized Lanthanides in Transparent Host Materials, in Handbook on the Physics and Chemistry of Rare Earths, Vol 5, K. A. Gschneidner and L. Eyring, Jr., eds., North Holland, New York (1982), p 632.

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(4) A. A. Kaminskii, Laser Crystals, Springer-Verlag, New York (1981), p 133.

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(7) S. H. Wemple and W. J. Tabor, Refractive Index Behavior of Garnets, J. Appl. Phys. 44 (1973), 1395.

(8) C. A. Morrison and R. P. Leavitt, Crystal Field Analysis of Triply Ionized Rare Earth Ions in Lanthanum Trifluoride, J. Chem. Phys. 71 (1979), 2366.

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(10) C. D. Brandle and R. L. Barns, Crystal Stoichiometry and Growth of Rare-Earth Garnets Containing Scandium, J. Cryst. Growth 20 (1979), 1.

(11) C. A. Morrison, Dipolar Contributions to the Crystal Field in Ionic Solids, Solid State Commun. 18 (1976), 153.

(12) C. A. Morrison, G. F. de Sá, and R. P. Leavitt, Self-Induced Multipole Contribution to the Single-Electron Crystal Field, J. Chem. Phys. 76 (1982), 3899.

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(13) D. E. Wortman, C. A. Morrison, and N. Karayianis, Rare Earth Ion-Host Lattice Interactions: 11. Lanthanides in $Y_3Al_5O_{12}$, Harry Diamond Laboratories, HDL-TR-1773 (August 1976).

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(15) C. A. Morrison, N. Karayianis, and D. E. Wortman, Rare Earth Ion-Host Lattice Interactions: 4. Predicting Spectra and Intensities of Lanthanides in Crystals, Harry Diamond Laboratories, HDL-TR-1816 (June 1977).

APPENDIX A.--COMPUTER OUTPUT

Detailed intensity (line-to-line) and g-factor calculations have been performed, and the results are attached in the form of microfiche copies of computer printouts for each ion in the lanthanide series, from Ce^{3+} to Yb^{3+}. In this appendix, we describe the contents of the computer printouts and present excerpts from them.

The computer printout for each ion presents the following information, in sequence, as follows:

(1) even-k crystal-field parameters, centroid parameters, and crystal-field-split energy levels;

(2) approximate Judd-Ofelt intensity calculations (no J mixing) including the Judd-Ofelt parameters, multiplet-to-multiplet line strengths, lifetimes, and branching ratios;

(3) full Judd-Ofelt squared matrix elements for π (E parallel to D_2 axis) and σ (E perpendicular to D_2 axis) between all crystal-field-split levels;

(4) a summary of the full Judd-Ofelt calculations (J mixing included), including multiplet-to-multiplet line strengths, lifetimes, and branching ratios;

(5) approximate magnetic-dipole intensity calculations (no J mixing), including multiplet-to-multiplet line strengths, lifetimes, and branching ratios;

(6) full magnetic-dipole squared matrix elements for σ (B parallel to D_2 axis) and π (B perpendicular to D_2 axis) between all crystal-field-split levels;

(7) a summary of the full magnetic-dipole calculations (J mixing included), including multiplet-to-multiplet line strengths, lifetimes, and branching ratios; and

(8) g factors (for an odd number of f electrons).

An excerpt of the energy level table for Pr^{3+} is given in table A-1. The crystal-field-split levels are numbered in sequence, beginning with the ground state (these sequence numbers are used later as identifiers in the line-to-line intensity calculations). The "PCT. PURE" column gives an indication of the amount of J mixing by the crystal field. The crystal quantum number column ("2MU") identifies, for an even number of f electrons, the irreducible representation of C_2 to which a level belongs; levels with $2\mu = 0$ are Γ_1 and levels with $2\mu = 2$ are Γ_2. For an odd number of electrons, all levels are

APPENDIX A

Kramers doublets with $2\mu = 1$ ($\Gamma_{3,4}$). The theoretical energy levels ("THEOR. ENERGY") correspond to those obtained using aqueous free-ion parameters.[1] (The "EXP. ENERGY" column is not relevant to this discussion.)

TABLE A-1. SAMPLE OF ENERGY LEVELS TABLE FROM COMPUTER OUTPUT FOR Pr^{3+} IN $Gd_3Sc_2Ga_3O_{12}$

FREE ION	PCT PURE	2MU	THEOR. ENERGY	EXP. ENERGY
1 3H 4	99.9	0	0.0	0.0
2 3H 4	99.8	0	38.4	0.0
3 3H 4	99.6	2	44.8	0.0
4 3H 4	98.5	0	452.8	0.0
5 3H 4	96.1	0	474.6	0.0
6 3H 4	95.8	2	507.4	0.0
7 3H 4	95.7	2	516.4	0.0
8 3H 4	94.4	2	717.2	0.0
9 3H 4	94.6	0	731.2	0.0
64 1D 2	99.9	2	16733.5	0.0
65 1D 2	99.9	0	16746.3	0.0
66 1D 2	99.9	0	17273.2	0.0
67 1D 2	99.9	0	17438.5	0.0
68 1D 2	99.8	2	17458.4	0.0

A sample of the computer printout for the approximate Judd-Ofelt calculations for Pr^{3+} is given in table A-2. In the table, the upper right elements give the multiplet-to-multiplet line strengths in units of square angstroms. Thus, for instance, the total line strength for the $^3H_5 \rightarrow {}^3F_3$ transition is 5.0×10^{-5} $Å^2$. The lower left elements in the table give the branching ratios for spontaneous emission, assuming that all levels within a multiplet are equally populated. The branching ratios, for example, for emission from the $^1D_2$ level are as follows:

0.06 for $^1D_2 \rightarrow {}^3F_4$,
0.0069 for $^1D_2 \rightarrow {}^3F_3$,
0.049 for $^1D_2 \rightarrow {}^3F_2$,
0.081 for $^1D_2 \rightarrow {}^3H_6$,
0.0063 for $^1D_2 \rightarrow {}^3H_5$, and
0.72 for $^1D_2 \rightarrow {}^3H_4$.

For a given initial state, all the branching ratios add up to unity. The calculation of the branching ratios neglects the dependence of the index of

[1] *W. T. Carnall, P. R. Fields, and K. Rajnak, Electronic Levels in the Trivalent Lanthanide Aquo Ions. Pr^{3+}, Nd^{3+}, Sm^{3+}, Dy^{3+}, Ho^{3+}, Er^{3+}, and Tm^{3+}, J. Chem. Phys. 49 (1968), 4412.*

refraction on frequency. The diagonal elements in the table give the lifetimes of the excited multiplets, again assuming equal populations of the initial sublevels. The quoted lifetimes are in seconds and should be divided by $n(n^2 + 2)^2/9$, where n is the index of refraction.

TABLE A-2. SAMPLE OF COMPUTER PRINTOUT SUMMARY OF ELECTRIC-DIPOLE TRANSITION PROBABILITY CALCULATIONS FOR Pr^{3+} IN $Gd_3Sc_2Ga_3O_{12}$ USING APPROXIMATE JUDD-OFELT THEORY

	3H 4	3H 5	3H 6	3F 2	3F 3	3F 4	1G 4	1D 2
3H 4	0.0	7.1E-04	1.6E-04	1.9E-04	8.3E-04	5.5E-04	3.1E-05	6.1E-05
3H 5	1.0E+00	2.1E-01	7.5E-04	7.8E-04	5.0E-05	5.3E-04	4.9E-04	8.1E-07
3H 6	6.3E-01	3.7E-01	8.9E-02	3.4E-04	9.9E-04	6.0E-04	3.2E-04	1.7E-05
3F 2	5.7E-01	4.3E-01	2.8E-03	1.7E-02	7.3E-06	1.0E-04	9.9E-06	1.2E-05
3F 3	9.5E-01	1.6E-02	3.6E-02	7.3E-05	4.4E-03	1.6E-05	5.9E-05	2.4E-06
3F 4	7.4E-01	2.2E-01	3.8E-02	2.3E-03	6.4E-06	5.4E-03	4.2E-04	2.4E-05
1G 4	9.3E-02	7.0E-01	1.6E-01	3.4E-03	7.7E-03	3.6E-02	4.1E-03	9.2E-05
1D 2	7.2E-01	6.3E-03	8.1E-02	4.9E-02	6.9E-03	6.0E-02	7.9E-02	1.8E-03

An excerpt from the squared matrix-element table is given in table A-3 for the π-spectrum, $^3H_4 \rightarrow {}^1D_2$ line-to-line electric-dipole transitions. It should be kept in mind that the polarizations referred to in this and the following table are with respect to the individual C_2 axes of the sites, and not the c-axis of the crystal. In table A-3, one number is presented for each transition, the squared matrix element p_z^2 of the z component of the electric dipole operator, in units of square angstroms.

TABLE A-3. EXCERPTS FROM COMPUTER OUTPUT FOR Pr^{3+}:$Gd_3Sc_2Ga_3O_{12}$ LINE-TO-LINE π ELECTRIC-DIPOLE TRANSITION PROBABILITY TABLE, FOR $^3H_4 \rightarrow {}^1D_2$ TRANSITIONS WITH $2\mu = 0 \rightarrow 2\mu = 0$ AND $2\mu = 2 \rightarrow 2\mu = 2$

$2\mu = 0 \rightarrow 2\mu = 0$			
		65 1D 2	6667 1D 21D 2
1 3H 4	3.568E-07	5.986E-06	8.124E-19
2 3H 4	1.921E-18	6.741E-18	6.936E-08
4 3H 4	8.742E-19	3.210E-20	6.083E-07
5 3H 4	3.344E-08	5.293E-07	6.175E-19
9 3H 4	3.136E-18	1.374E-18	4.265E-06

$2\mu = 2 \rightarrow 2\mu = 2$		
	64 1D 2	68 1D 2
3 3H 4	6.741E-06	1.608E-19
6 3H 4	4.875E-07	3.644E-18
7 3H 4	1.652E-17	8.572E-08
8 3H 4	2.502E-21	2.134E-06

APPENDIX A

Table A-4 shows excerpts from the squared matrix elements table for the σ-spectrum, $^3H_4 \rightarrow {}^1D_2$ electric-dipole transitions. Again, the polarization (σ) is with respect to the site D_2 axis. For each transition, three numbers are presented in the table: $P^2_{xy}(max)$, $P^2_{xy}(min)$, and θ_m.

TABLE A-4. EXCERPTS FROM COMPUTER OUTPUT FOR $Pr^{3+}:Gd_3Sc_2Ga_3O_{12}$ LINE-TO-LINE σ ELECTRIC-DIPOLE TRANSITION PROBABILITY TABLE, FOR $^3H_4 \rightarrow {}^1D_2$ TRANSITIONS WITH $2\mu = 0 \rightarrow 2\mu = 2$ AND $2\mu = 2 \rightarrow 2\mu = 0$

$2\mu = 0 \rightarrow 2\mu = 2$					
		1 3H 4	2 3H 4	4 3H 4	5 3H 4	9 3H 4
64	1D 2	4.686E-06	2.211E-07	3.440E-09	1.146E-06	6.598E-08
		0.0	0.0	0.0	0.0	0.0
		0.0	0.0	0.0	0.0	0.0
68	1D 2	3.062E-06	1.140E-07	5.466E-07	2.875E-07	3.126E-06
		4.547E-13	0.0	5.684E-14	2.842E-14	0.0
		90.0	90.0	0.0	90.0	0.0

$2\mu = 2 \rightarrow 2\mu = 0$				
		65 1D 2	66 1D 2	67 1D 2
3	3H 4	2.772E-07	5.163E-06	3.299E-06
		2.842E-14	4.547E-13	4.547E-13
		0.0	0.0	90.00
6	3H 4	1.993E-09	9.950E-08	1.874E-07
		1.110E-16	0.0	-2.842E-14
		0.0	0.0	90.00
7	3H 4	4.879E-07	3.618E-06	1.553E-06
		8.527E-14	0.0	0.0
		90.00	90.00	0.0
8	3H 4	2.593E-06	5.663E-07	2.482E-07
		0.0	2.842E-14	2.842E-14
		90.00	90.00	0.0

The remaining computer printout for intensity calculations consists of multiplet-to-multiplet tables and line-to-line tables, as described above. These tables have the same format as those already described. It should be remembered that, for the magnetic-dipole tables, π and σ are reversed; that is, σ corresponds to the B vector along z, and π corresponds to the B vector perpendicular to z. Also, for the magnetic-dipole transitions, the radiative lifetime is to be divided by n^3, where n is the index of refraction.

For an odd number of electrons, all the levels are Kramers doublets, and g factors have been computed. The g tensor can be characterized by four numbers: $g_\parallel$ (B parallel to z), $g_{\perp 1}$ and $g_{\perp 2}$ (maximum and minimum values of $g_\perp$ for B in the x-y plane, respectively), and θ_m (the angle in the x-y plane for which $g_\perp$ is a maximum). These are presented on the last page of the computer output.

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